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Computational model for power optimization of piezoelectric vibration energy harvesters with material homogenization

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ABSTRACT

Piezoelectric vibration power harvesters are being studied in the literature since they have high energy conversion from mechanical vibrations. A computational model that optimizes piezoelectric vibration energy harvester output power using homogenization of piezoelectric material is presented in this work. This computational model allows piezoelectric material tailoring to create piezoelectric vibrational energy harvesters capable of producing higher electrical power. The materials considered in the study are single crystal and polycrystals of $BaTiO_3$ and PZN-4.5%PT, and piezopolymer PVDF-TrFE and the piezocomposites of these materials. The computational model is used to optimize the harvester power output of the unimorph vibration harvester configuration. The harvesters are modelled using the finite element method which is validated comparing analytical results for four traditional harvester configurations, *viz.*, unimorph, bimorph, longitudinal generator and transverse generator. Single crystals, polycrystals and piezocomposites made by piezoceramic and piezopolymer materials are considered in the optimization procedure. Polycrystalline and piezocomposite properties are computed through a computational model based in the homogenization theory, which is implemented using the finite element method. Electrical resistance is used as the surrogate for the electrical machine connected to the harvesters. The design variables considered are the crystal orientation for single crystal materials, microstructural orientation distribution of the grains for polycrystalline materials, the piezoceramic material volume fraction and piezopolymer orientation for piezocomposites and/or the circuit resistance. A simulated annealing algorithm based in Metropolis algorithm is used as the optimizer. Several examples are presented and discussed considering excitations near as well as far away from resonance frequency. Harvesters with material composites having optimal material configurations that deliver enhanced electrical power have been identified.

1. Introduction

Nowadays the development of low power electronics devices encourages the use of ambient power harvesting devices. Among them, piezoelectric harvesters convert ambient mechanical vibrations into useable electric power. The recent advancements in materials and circuits technologies plus low power consumption devices encourage the use of piezoelectric materials for vibrations energy harvesting [1–4]. The piezoelectric harvesters use the piezoelectric effect to convert directly mechanical vibrations into electrical energy and tap this energy by connecting the harvester electrodes with an electric circuit. The use of optimization techniques to design the material layouts of piezoelectric systems for actuation or resonator systems have been studied previously [3–5]. Various models including beam energy harvester frequency self-tuning have been proposed to study piezoelectric vibrations harvesters [5–8] being typically 1D or 2D, ignoring material anisotropy effects since the orientation of the piezoelectric materials is kept constant. Based on these models, methods to improve piezoelectric vibration harvester power output were developed. Most piezoelectric energy harvesting approaches to date focus on the electromechanics of the piezoelectric transduction and use a transient or steady-state vibrational signature, usually at resonance, as input for the base excitation of the piezoelectric harvesting structure which is often coupled one-way to a simple external harvesting circuit [5–7]. It is shown that many of the outstanding problems associated with piezoelectric transducers, including mechanical stability under large stresses, electrical breakdown of the material under high fields or reduction in efficiency due to dielectric losses and depolarization can be overcome by smart design and better material selection [3]. Here, in this work the material anisotropy at the microstructural level is included in the piezoelectric harvester model and its impact in power output is

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studied. A 3D modelling of piezoelectric vibration harvester is necessary to study the effects of material anisotropy comprehensively. A group of piezoelectric materials typically used for energy harvesting are the piezoelectric ceramics [1,2]. Among these materials lead zirconate titanate (PZT) and barium titanate ($BaTiO_3$) exhibit very high dielectric and piezoelectric properties being suitable for piezoelectric energy harvesters [1,2]. The piezoelectric materials can be crystalline solids either with a single crystalline or polycrystalline microstructure. The polycrystalline solid grain (or crystallite) orientations plus shape and grain boundaries can be known using X-ray diffraction contrast tomography [9,10]. Conventional methods to characterize the polycrystalline piezoelectric ceramic properties can be found, e.g., in [11–13]. Previous works [14] have shown that the value of piezoelectric and dielectric constants can change with grain size for $BaTiO_3$ and with grain boundary thickness [15] for $PbTiO_3$.

The piezoelectric materials properties used in harvesters can be tailored, for example, by building a piezocomposite microstructure [16,17] of piezoelectric rods and a polymer matrix, doping piezoelectric material [18–20] or creating a composite microstructure [21–23]. In this work we will address the tailoring of piezoelectric material properties for unimorph configuration as an example of the computational model capabilities. For this purpose, a computational model based in finite elements is applied to piezoelectric harvesters while optimization combined with homogenization is employed for the tailoring of the material. The finite element method has been used successfully to model piezoelectric harvesters and shows a good approximation to experimental results [6,24–27] showing a maximum relative difference of harvesters displacement 14.3% and of peak frequency 12.5%. For the material tailoring, two different cases will be considered, namely the single crystal and the polycrystal. For the polycrystalline case, the characterization of the macroscopic piezoelectric properties is made using the asymptotic homogenization method for piezoelectricity with a suitable representative volume element (RVE), (see, for example, Galka et al. [28], Silva et al. [21]). Here, Ref. [22] is followed for its application to polycrystalline case. The homogenization method has been successfully used to model several different physical problems [21–23,28–30] and has been shown to provide good agreement both computationally and experimentally [31]. The material tailoring consists in finding an optimal orientation for piezoelectric single crystalline materials, or an optimal statistical distribution of grain orientation for the polycrystalline case [22]. Also, this will be applied to piezoceramics and composites of piezoceramics and piezopolymers. Though piezopolymers [32,33] have lower piezoelectric coupling properties than piezoceramics, they however possess significantly higher flexibility. This will enable the possibility to produce a composite piezoelectric material with high piezoelectric properties and good flexibility, being suitable for low wind speed energy harvesters [34], automobile tire harvesters [35], etc. Here we have assumed that the crystal orientation distribution in a polycrystalline piezoelectric ceramic material is a Gaussian or normal distribution as it is treated in Ref. [22].

The main contribution of this work is the development of a computational model for the optimization of piezoelectric harvesters. This model incorporates a simulated annealing optimization algorithm, an in house finite element computational tool for determining the homogenized piezoelectric material properties, and commercial finite element software for the harvester modelling. Several examples are presented to show the applicability of the model. The significance of this work is the versatility of the present 3D model of the transducer in the potential future applications that envisage the harvester configuration to be suitable to any useful shapes or geometries. Hence in order to suit the integration of the harvester to devices of various shapes and geometries, a 3D transducer that harvest mechanical energy is imperative.

This paper is divided into 12 sections. In Sections 2–9 the problem formulation is presented, describing all the aspects involving the problem formulation, namely the harvested power, the homogenization equations, the harvester geometry, the piezoelectric harvester configurations, the finite element problem, the optimization procedure, the material properties and the finite element model validation. In Section 10 the unimorph harvester configuration is optimized with respect to material orientation and resistance of the electric circuit, for excitation far away from resonance. A piezocomposite is also considered in this situation. In Section 11 the previous unimorph harvester configuration is tuned for ambient vibrations, such that it operates near a resonance/natural frequency. This new harvester is named *UniT* and its power output is optimized for a collection of excitation frequencies around *UniT* natural frequency, considering different piezoelectric materials and also piezocomposites. In Section 12 conclusions and future work are presented.

2. Problem formulation

To model the piezoelectric harvester, the classic electro-elastic equations will be assumed in its linearized form, for infinitesimal strains and potential gradients (see e.g. [36]). In piezoelectric vibration energy harvesters typically electrodes are used to link the piezoelectric material to the electric circuit as presented in Fig. 1. For the harvester shown in Fig. 1, these equations can be summarized as:

$$\begin{cases} T_{jk,j} = \rho \ddot{u}_k \ in\ \Omega \\ D_{i,i} = 0\ in\ \Omega \\ S_{ij} = \frac{u_{i,j}+u_{j,i}}{2} \\ E_i = -\phi_{,i} \\ T_{ij} = C^E_{ijkl} S_{kl} - e_{kij} E_k \\ D_i = e_{ikl} S_{kl} + \varepsilon^S_{ik} E_k \\ \Delta\phi = RI \\ u_i = \overline{u_i}\ on\ \Gamma_u \\ t_i = T_{ji} n_j\ on\ \Gamma_T \\ \phi = \overline{\phi_1}\ on\ \Gamma_{\phi_1} \\ \phi = \overline{\phi_2}\ on\ \Gamma_{\phi_2} \\ D_j n_j = 0\ on\ \Gamma_D \end{cases} \tag{1}$$

where, in the equation of motion, T_{ji} is the stress tensor, ρ material density and u_k the displacement; in the charge equation, D_i is the electrical displacement; S_{ij} is the infinitesimal strain, E_i is the electrical field and ϕ the potential . In the linear constitutive equations, C^E_{ijkl} is the stiffness measured at constant electrical field, e_{kij} is the piezoelectric stress coefficients and ε^S_{ik} is the dielectric matrix measured at constant strain. The circuit equation relates the potential difference with the resistance R and the electric current I through it. Then for the boundary conditions, there are the usual prescribed displacement u_{oi} and traction t_i conditions on Γ_u and Γ_T, respectively, and the prescribed potential $\overline{\phi_i}$ and charge condition $q = 0$ on Γ_{ϕ_i} and Γ_D respectively as it can be seen in Fig. 1. Note that the Γ_{ϕ_i} surfaces represent the electrode surfaces, and that the harvester surface $\Gamma = \Gamma_{\phi_1} \cup \Gamma_{\phi_2} \cup \Gamma_D = \Gamma_u \cup \Gamma_T$. Einstein convention on summation about dummy indices is followed in this paper and the notation $\alpha_{i,j}$ represents partial derivatives $\frac{\partial \alpha_i}{\partial x_j}$ with respect to spatial coordinates. Each electrode has a constant electrical potential on a surface Γ_{ϕ_i}. The total free electrical charge crossing Γ_{ϕ_i} is given by expression,